10/513699

Connecting via Winsock to STN

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS 1   Web Page for STN Seminar Schedule - N. America
 NEWS 2 DEC 01 ChemPort single article sales feature unavailable
 NEWS 3 APR 03 CAS coverage of exemplified prophetic substances
                 enhanced
 NEWS 4 APR 07 STN is raising the limits on saved answers
 NEWS 5 APR 24 CA/CAplus now has more comprehensive patent assignee
                 information
 NEWS 6 APR 26 USPATFULL and USPAT2 enhanced with patent
                 assignment/reassignment information
 NEWS 7 APR 28 CAS patent authority coverage expanded
 NEWS 8 APR 28 ENCOMPLIT/ENCOMPLIT2 search fields enhanced
 NEWS 9 APR 28 Limits doubled for structure searching in CAS
                 REGISTRY
 NEWS 10 MAY 08 STN Express, Version 8.4, now available
 NEWS 11 MAY 11 STN on the Web enhanced
 NEWS 12 MAY 11 BEILSTEIN substance information now available on
                 STN Easy
 NEWS 13 MAY 14 DGENE, PCTGEN and USGENE enhanced with increased
                 limits for exact sequence match searches and
                 introduction of free HIT display format
 NEWS 14 MAY 15 INPADOCDB and INPAFAMDB enhanced with Chinese legal
                 status data
 NEWS 15 MAY 28 CAS databases on STN enhanced with NANO super role in
                 records back to 1992
 NEWS 16 JUN 01 CAS REGISTRY Source of Registration (SR) searching
                 enhanced now on STN

 NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
              AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

 NEWS HOURS   STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN   Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that
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  and other penalties.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:06:12 ON 09 JUN 2009

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                   ENTRY   SESSION
FULL ESTIMATED COST   0.22   0.22

FILE 'REGISTRY' ENTERED AT 16:06:33 ON 09 JUN 2009
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STRUCTURE FILE UPDATES: 8 JUN 2009 HIGHEST RN 1154048-98-2
DICTIONARY FILE UPDATES: 8 JUN 2009 HIGHEST RN 1154048-98-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file casreact
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                   ENTRY   SESSION
FULL ESTIMATED COST   0.48   0.70

FILE 'CASREACT' ENTERED AT 16:06:38 ON 09 JUN 2009
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FILE CONTENT:1840 - 8 Jun 2009 VOL 150 ISS 24

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*   *
*   CASREACT now has more than 16.5 million reactions   *

<12/04/2007>   Erich Leese

```
=>
Uploading C:\Program Files\Stnexp\Queries\10579106stereounspecific.str
```



```
chain nodes :
21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41
42  43  44  45
ring nodes :
1   2   3   4   5   6   7   8   9   10  11  12  13  14  15  16  17  18  19  20
chain bonds :
1-35  4-34  5-21  5-32  8-38  9-37  10-44  12-39  13-36  14-45  18-26  18-33  21-22
 21-25  22-23  22-24  26-27  26-29  27-28  27-30  28-31  38-40  38-41  39-42  39-43

ring bonds :
1-2   1-6   2-3   2-7   3-4   3-10  4-5   5-6   7-8   8-9   9-10  11-12  11-16  12-13  13-14
 14-15  15-16  15-17  16-20  17-18  18-19  19-20
exact/norm bonds :
1-2   1-6   2-3   2-7   3-4   3-10  4-5   5-6   7-8   8-9   8-38  9-10  10-44  11-12  11-16
12-13  12-39  13-14  14-15  14-45  21-25  22-24  26-29  27-30  28-31
exact bonds :
1-35  4-34  5-21  5-32  9-37  13-36  18-26  18-33  21-22  22-23  26-27  27-28
38-40  38-41  39-42  39-43
normalized bonds :
15-16  15-17  16-20  17-18  18-19  19-20
isolated ring systems :
containing 1 : 11 :


Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom
20:Atom   21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
28:CLASS   29:CLASS   30:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS
36:CLASS   37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:CLASS   43:CLASS
44:CLASS   45:CLASS
fragments assigned product role:
containing 1
```
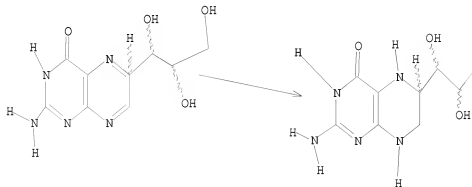
fragments assigned reactant/reagent role:
containing 11

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 122.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:07:15 FILE 'CASREACT'
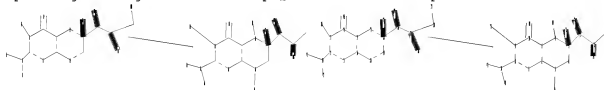SCREENING COMPLETE -   29 REACTIONS TO VERIFY FROM   9 DOCUMENTS

100.0% DONE   29 VERIFIED   0 HIT RXNS   0 DOCS
SEARCH TIME: 00.00.01

L2   0 SEA SSS FUL L1 (0 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\10579106unspecified bonds.str

chain nodes :
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41
42 43 44 45
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :

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```
1-35   4-34   5-21   5-32   8-38   9-37   10-44  12-39  13-36  14-45  18-26  18-33  21-22
 21-25  22-23  22-24  26-27  26-29  27-28  27-30  28-31  38-40  38-41  39-42  39-43

ring bonds :
1-2   1-6   2-3   2-7   3-4   3-10   4-5   5-6   7-8   8-9   9-10   11-12  11-16  12-13  13-14
 14-15  15-16  15-17  16-20  17-18  18-19  19-20
exact/norm bonds :
1-2   1-6   2-3   2-7   3-4   3-10   4-5   5-6   7-8   8-9   8-38   9-10   10-44  11-12  11-16
12-13  12-39  13-14  14-15  14-45  15-16  15-17  16-20  17-18  18-19  19-20  21-25
22-24  26-29  27-30  28-31
exact bonds :
1-35   4-34   5-21   5-32   9-37   13-36  18-26  18-33  21-22  22-23  26-27  27-28
38-40  38-41  39-42  39-43
isolated ring systems :
containing 1 : 11 :



Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   18:Atom   19:Atom
20:Atom   21:CLASS   22:CLASS   23:CLASS   24:CLASS   25:CLASS   26:CLASS   27:CLASS
28:CLASS   29:CLASS   30:CLASS   31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS
36:CLASS   37:CLASS   38:CLASS   39:CLASS   40:CLASS   41:CLASS   42:CLASS   43:CLASS
44:CLASS   45:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 11




L3      STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3              STR
```
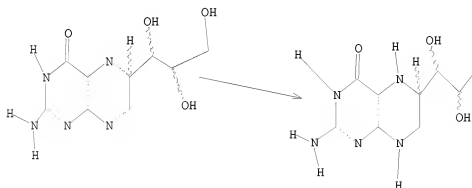


```
Structure attributes must be viewed using STN Express query preparation.


=> s l3 full
```

THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 122.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:08:50 FILE 'CASREACT'
SCREENING COMPLETE -   29 REACTIONS TO VERIFY FROM   9 DOCUMENTS

100.0% DONE   29 VERIFIED   0 HIT RXNS   0 DOCS
SEARCH TIME: 00.00.01

L4   0 SEA SSS FUL L3 (0 REACTIONS)

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                     ENTRY   SESSION
FULL ESTIMATED COST   247.22   247.92

FILE 'REGISTRY' ENTERED AT 16:09:12 ON 09 JUN 2009
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STRUCTURE FILE UPDATES: 8 JUN 2009 HIGHEST RN 1154048-98-2
DICTIONARY FILE UPDATES: 8 JUN 2009 HIGHEST RN 1154048-98-2

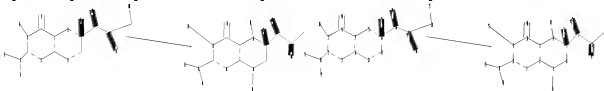New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10579106unspecified bonds.str

chain nodes :
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41
42 43 44 45
ring nodes :
1   2   3   4   5   6   7   8   9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
1-35 4-34 5-21 5-32 8-38 9-37 10-44 12-39 13-36 14-45 18-26 18-33 21-22
 21-25 22-23 22-24 26-27 26-29 27-28 27-30 28-31 38-40 38-41 39-42 39-43

```
ring bonds :
1-2  1-6  2-3  2-7  3-4  3-10  4-5  5-6  7-8  8-9  9-10  11-12  11-16  12-13  13-14
 14-15  15-16  15-17  16-20  17-18  18-19  19-20
exact/norm bonds :
1-2  1-6  2-3  2-7  3-4  3-10  4-5  5-6  7-8  8-9  8-38  9-10  10-44  11-12  11-16
12-13  12-39  13-14  14-15  14-45  15-16  15-17  16-20  17-18  18-19  19-20  21-25
22-24  26-29  27-30  28-31
exact bonds :
1-35  4-34  5-21  5-32  9-37  13-36  18-26  18-33  21-22  22-23  26-27  27-28
38-40  38-41  39-42  39-43
isolated ring systems :
containing 1 : 11 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
28:CLASS  29:CLASS  30:CLASS  31:CLASS  32:CLASS  33:CLASS  34:CLASS  35:CLASS
36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS  41:CLASS  42:CLASS  43:CLASS
44:CLASS  45:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 11




L5      STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5              STR
```
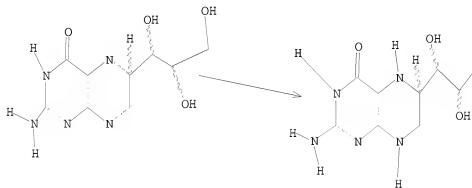


```
Structure attributes must be viewed using STN Express query preparation.


=> s l5 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
```

<12/04/2007>   Erich Leese

```
MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE
COMMAND INTERRUPTED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> file casreact
COST IN U.S. DOLLARS                               SINCE FILE      TOTAL
                                                       ENTRY     SESSION
FULL ESTIMATED COST                                      2.40     250.32

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FILE CONTENT:1840 - 8 Jun 2009 VOL 150 ISS 24

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*************************************************************
*                                                           *
*      CASREACT now has more than 16.5 million reactions    *
*                                                           *
*************************************************************

CASREACT contains reactions from CAS and from: ZIC/VINITI database
(1974-1999) provided by InfoChem; INPI data prior to 1986;
Biotransformations database compiled under the direction of
Professor Dr. Klaus Kieslich; organic reactions, portions copyright
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This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10579106last.str
```
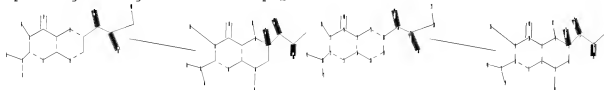


```
chain nodes :
21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40  41
42  43  44
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20
chain bonds :
```

```
1-34   4-33   5-21   5-32   8-37   9-36   10-43  12-38  13-35  14-44  18-26  21-22  21-25
 22-23  22-24  26-27  26-29  27-28  27-30  28-31  37-39  37-40  38-41  38-42
ring bonds :
1-2   1-6   2-3   2-7   3-4   3-10  4-5   5-6   7-8   8-9   9-10  11-12  11-16  12-13  13-14
 14-15  15-16  15-17  16-20  17-18  18-19  19-20
exact/norm bonds :
1-2   1-6   2-3   2-7   3-4   3-10  4-5   5-6   7-8   8-9   8-37  9-10  10-43  11-12  11-16
12-13  12-38  13-14  14-15  14-44  15-16  15-17  16-20  17-18  18-19  19-20  21-25
22-24  26-29  27-30  28-31
exact bonds :
1-34   4-33   5-21   5-32   9-36   13-35  18-26  21-22  22-23  26-27  27-28  37-39
37-40  38-41  38-42
isolated ring systems :
containing 1 : 11 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
28:CLASS  29:CLASS  30:CLASS  31:CLASS  32:CLASS  33:CLASS  34:CLASS  35:CLASS
36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS  41:CLASS  42:CLASS  43:CLASS
44:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 11




L6      STRUCTURE UPLOADED

=> d l6
L6 HAS NO ANSWERS
L6              STR
```
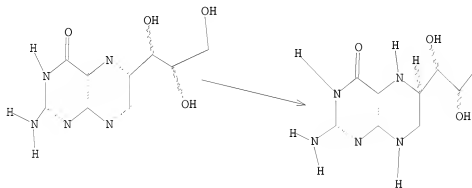


```
Structure attributes must be viewed using STN Express query preparation.


=> s l6 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 122.65 U.S. DOLLARS
```

```
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:12:42 FILE 'CASREACT'
SCREENING COMPLETE -      29 REACTIONS TO VERIFY FROM      9 DOCUMENTS

100.0% DONE      29 VERIFIED      4 HIT RXNS                      3 DOCS
SEARCH TIME: 00.00.01

L7          3 SEA SSS FUL L6 (     4 REACTIONS)

=> d ibib abs hitstr tot
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB ------- AN, plus Bibliographic Data (original)
OIBIB ------ OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
```

```
              HIT, PATH, SPATH reactions. Labels reactions that have
              incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
              path".  Displays all hit reactions, except those
              whose steps are totally included within another hit
              reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
              path".  Displays all single step reactions which
              contain a hit substance.  Also displays those
              multistep reactions that have a hit substance in both
              the first and last steps of the reaction, except for
              those hit reactions whose steps are totally included
              within another hit reaction which is displayed
```
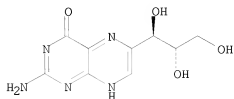
To display a particular field or fields, enter the display field
codes. For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>). Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD. The information is displayed in the same order
as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):.
THE ESTIMATED COST FOR THIS REQUEST IS 9.18 U.S. DOLLARS
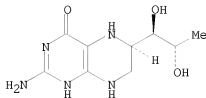DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

RX(13) OF 15 - 3 STEPS

1. Me2NCH(OEt)2, DMF
2. PhSSPh, PBu3,
   AcNMe2
3.1. Ni, H2, EtOH
3.2. HCl

stereoisomers
16%

REF: PCT Int. Appl., 2005049614, 02 Jun 2005
NOTE: 3) stereoselective, Raney nickel was used
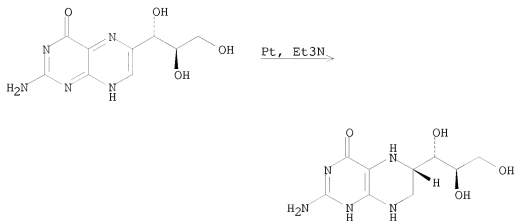CON: STEP(1) 6 hours, room temperature
      STEP(2.1) room temperature; 4 hours, room temperature
      STEP(3.1) room temperature; 17 hours, room temperature, 5 bar

RX(1) OF 1

Pt, Et3N

2 HCl

REF: Jpn. Kokai Tokkyo Koho, 07188233, 25 Jul 1995, Heisei
NOTE: at 0-5.degree., 100 Kg/cm2 for 20 min

RX(6) OF 7
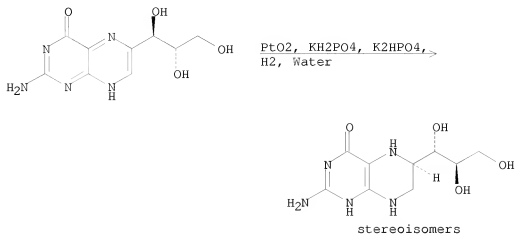

PtO2, KH2PO4, K2HPO4,
H2, Water

stereoisomers

REF: Heterocycles, 23(12), 3115-20; 1985
NOTE: pH .gtoreq.10.8

```
=> s 17 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 122.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:13:45 FILE 'CASREACT'
SCREENING COMPLETE -      29 REACTIONS TO VERIFY FROM        9 DOCUMENTS

100.0% DONE      29 VERIFIED       4 HIT RXNS                      3 DOCS
SEARCH TIME: 00.00.01

L8          3 SEA SSS FUL L6 (      4 REACTIONS)

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THE ESTIMATED COST FOR THIS REQUEST IS 15.63 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y
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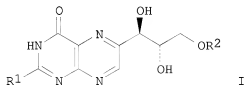
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L8    ANSWER 1 OF 3  CASREACT  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        143:7534  CASREACT
TITLE:                   Preparation of tetrahydrobiopterin and analogs of
                         tetrahydrobiopterin
INVENTOR(S):             Moser, Rudolf; Groehn, Viola; Schumacher, Andreas;
                         Martin, Pierre
PATENT ASSIGNEE(S):      Biomarin Pharmaceutical Inc., USA; Merck Eprova A.-G.
SOURCE:                  PCT Int. Appl., 55 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE            APPLICATION NO.  DATE
     ---------------   ----  --------        ---------------  --------
     WO 2005049614     A2    20050602        WO 2004-US38313  20041117
     WO 2005049614     A3    20070308
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW:  BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO,
             SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
     AU 2004290692     A1    20050602        AU 2004-290692   20041117
     CA 2545484        A1    20050602        CA 2004-2545484  20041117
     EP 1776364        A2    20070425        EP 2004-819154   20041117
         R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, HR, LT,
             LV, MK, YU
     JP 2007534637     T     20071129        JP 2006-539994   20041117
     US 20070244322    A1    20071018        US 2007-579106   20070216
PRIORITY APPLN. INFO.:                       US 2003-520367P  20031117
                                             US 2003-520368P  20031117
                                             WO 2004-US38313  20041117
OTHER SOURCE(S):         MARPAT 143:7534
GI
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AB    A process for the preparation of tetrahydrobiopterin and its analogs, e.g. I
      [R1 = alkylamino, arylamino, alkylthio, alkylaminomethyleneimino, R2 = H;
      R1 = alkylamino, alkylthio, Me2NCH:N, R2 = Me2CHEt2Si, (Me3CO)Ph2Si,
      MePh2Si, Me3CMe2Si, Me3C(MeO)PhSi, (Me3C)2MeSi, etc.], from neopterin
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and/or 6-substituted pterins with an improved yield and a high
stereoselectivity is disclosed. Also disclosed herein are novel
individual intermediates prepared in the preparation of tetrahydrobiopterin,
such
as selectively protected neopterin useful for the preparation of
tetrahydrobiopterin. As an example, L-neopterin was reacted with
DMF-acetal to give the 2-(dimethylamino)methylene derivative I (R1 = Me2NCH:N,
R2 = H) (II). II was then silylated to I (R2 = Me3CPh2Si) which could be
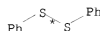deprotected to I (R1 = NH2).

RX(13) OF 15 COMPOSED OF RX(1), RX(5), RX(6)
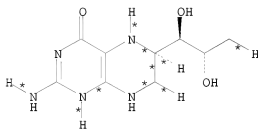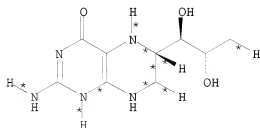RX(13)   2 A + 2 B + 2 N ===> R + S
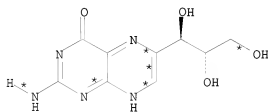
2 A
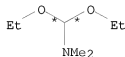
2 B

2 N

3
STEPS
⟹

R
YIELD 16%

S
YIELD 9%

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RX(1)     RCT  A 2277-43-2, B 1188-33-6
          PRO  C 852547-43-4
          SOL  68-12-2 DMF
          CON  6 hours, room temperature

RX(5)     RCT  C 852547-43-4, N 882-33-7
          RGT  P 998-40-3 PBu3
          PRO  O 852547-49-0
          SOL  127-19-5 AcNMe2
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) 4 hours, room temperature

RX(6)     RCT  O 852547-49-0

             STAGE(1)
                 RGT  T 1333-74-0 H2
                 CAT  7440-02-0 Ni
                 SOL  64-17-5 EtOH
                 CON  SUBSTAGE(1) room temperature
                      SUBSTAGE(2) 17 hours, room temperature, 5 bar

             STAGE(2)
                 RGT  U 7647-01-0 HCl

          PRO  R 62989-33-7, S 62961-57-3
          NTE  stereoselective, Raney nickel was used
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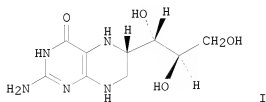
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L8    ANSWER 2 OF 3  CASREACT  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        123:256436  CASREACT
TITLE:                   Preparation of (6S)-tetrahydro-D-neopterin via
                         catalytic hydrogenation of D-neopterin.
INVENTOR(S):             Mochizuki, Naoki; Uemitsu, Nobuo
PATENT ASSIGNEE(S):      Asahi Breweries Ltd, Japan
SOURCE:                  Jpn. Kokai Tokkyo Koho, 3 pp.
                         CODEN: JKXXAF
DOCUMENT TYPE:           Patent
LANGUAGE:                Japanese
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

      PATENT NO.      KIND  DATE          APPLICATION NO.   DATE
      --------------- ----  --------      ---------------   --------
      JP 07188233     A     19950725      JP 1993-346845    19931227
      JP 2995448      B2    19991227
PRIORITY APPLN. INFO.:                    JP 1993-346845    19931227
GI
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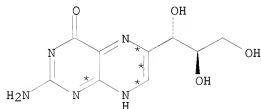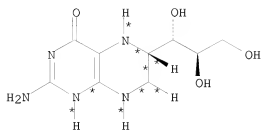

I

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AB    (6S)-tetrahydro-D-neopterin (I) is prepared via hydrogenation of D-neopterin
      under 80-120 Kg/cm2 pressure, pH 10-13.  Thus, D-neopterin, platinum, and
      Et3N were placed in an autoclave and the reaction mixture was maintained at
      0-5°, 100 Kg/cm2 for 20 min to give, after treatment with concentrated
      HCl, I dihydrochloride.


RX(1) OF 1    A  ===>  B
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A

(1)

● 2 HCl

B

RX(1)   RCT A 2009-64-5
          RGT C 121-44-8 Et3N
          PRO B 169219-49-2
          CAT 7440-06-4 Pt
          NTE at 0-5°, 100 Kg/cm2 for 20 min

L8   ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 105:208658 CASREACT
TITLE: Hydrogenation of biopterin and its analogs;
                        application for the convenient procedure of biopterin
                        cofactor and related 5,6,7,8-tetrahydropterins
AUTHOR(S):   Matsuura, Sadao; Murata, Shizuaki; Sugimoto, Takashi
CORPORATE SOURCE: Coll. Gen. Educ., Nagoya Univ., Nagoya, 464, Japan
SOURCE: Heterocycles (1985), 23(12), 3115-20
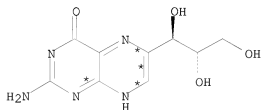   CODEN: HTCYAM; ISSN: 0385-5414
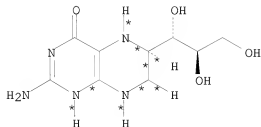DOCUMENT TYPE: Journal
LANGUAGE: English
AB   A large scale and stereoselective hydrogenation of biopterin to
     (6R)-5,6,7,8-tetrahydrobiopterin was achieved by using PtO2 catalyst at pH
     11.8. The procedure was applied for various hydroxyalkylpterins such as
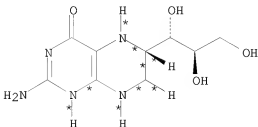   neopterin and diastereomers of biopterin.

RX(6) OF 7   2 S ===> T + U

2 S

                                        (6)
                                       ──────>

T   U

RX(6)   RCT S 2277-43-2
         RGT D 7778-77-0 KH2PO4, E 7758-11-4 K2HPO4, F 1333-74-0 H2
         PRO T 78737-51-6, U 78737-52-7
         CAT 1314-15-4 PtO2
         SOL 7732-18-5 Water
         NTE pH ≥10.8

10/513699

=> d his

    (FILE 'HOME' ENTERED AT 16:06:12 ON 09 JUN 2009)

    FILE 'REGISTRY' ENTERED AT 16:06:33 ON 09 JUN 2009

    FILE 'CASREACT' ENTERED AT 16:06:38 ON 09 JUN 2009
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L1              STRUCTURE UPLOADED
L2          0 S L1 FULL
L3              STRUCTURE UPLOADED
L4          0 S L3 FULL
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    FILE 'REGISTRY' ENTERED AT 16:09:12 ON 09 JUN 2009
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L5              STRUCTURE UPLOADED
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    FILE 'CASREACT' ENTERED AT 16:12:07 ON 09 JUN 2009
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L6              STRUCTURE UPLOADED
L7          3 S L6 FULL
L8          3 S L7 FULL
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	272.51	522.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-2.34

STN INTERNATIONAL LOGOFF AT 16:14:58 ON 09 JUN 2009

<12/04/2007>   Erich Leese